Mission Adaptable Chemical Sensor

(MACS)

PROPOSERS DAY CONFERENCE

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Part 1. Overview of Requirements

Mission-Adaptable Chemical Spectrometer (MACS)

Vision : Advanced, high performance sensor development for major threat identification

Objective: Develop a portable, ultra-sensitive (parts per trillion [ppt]) chemical sensor providing unambiguous simultaneous identification of multiple (~500) molecular species with low (<0.0001%) false-alarm rate.

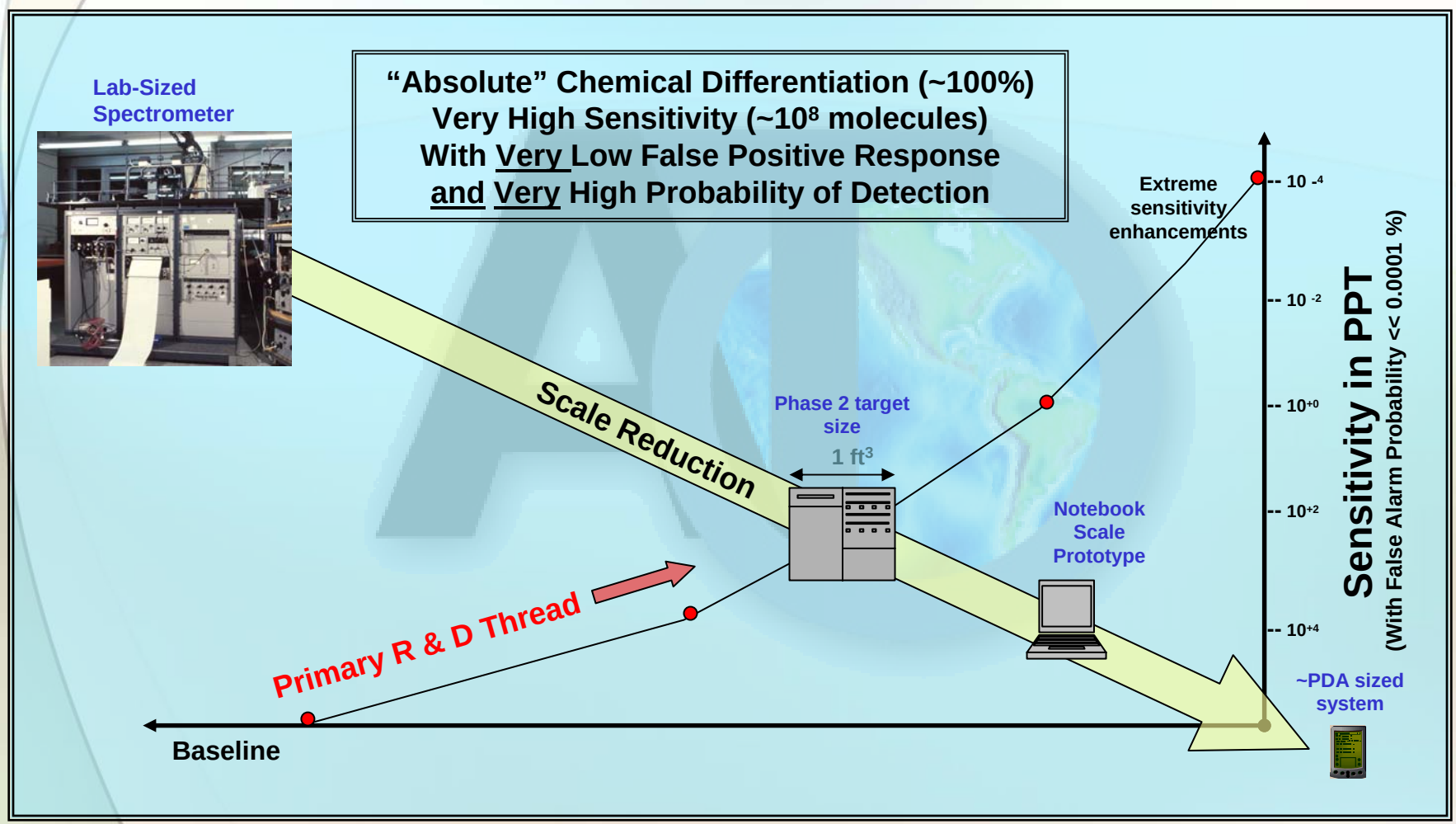
- **MACS has, theoretically, the highest probability of detection and lowest false-alarm rate of any other chemical sensor.**
  - **It can identify many 100s of chemical species simultaneously, at various concentration levels.**
  - **An accurate threat identification can be made by identifying its component chemical species under various atmospheric conditions.**

MACS Program – Concept
Why is MACS Fundamentally Different?

Capability of sampling the local atmosphere and determining the presence of chemical, biological, and explosives threats by means of their gaseous signatures.

- **Unambiguous identification of threats can be accomplished by the rapid, simultaneous identification of many gaseous chemicals in a cluttered atmospheric environment.**
- **The ability to perform the analysis quickly and with unprecedented specificity across almost any range of exposures and environments.**
- **MACS does not require combination / hyphenation with other analytical techniques to produce its very favorable ROCs, nor is it an engineering evolution, similar to other evolutions that combine mature sensor approaches such as GC, MS, IR, SAW, IMS, etc.**

MACS Program - Overview



MACs – Primary Goals and Milestones

Capability to quickly identify all relevant CWA's, TIC's and TIM's in the presence of a cluttered background.

<u>Phase I performance goals</u> (in atmospheric clutter)

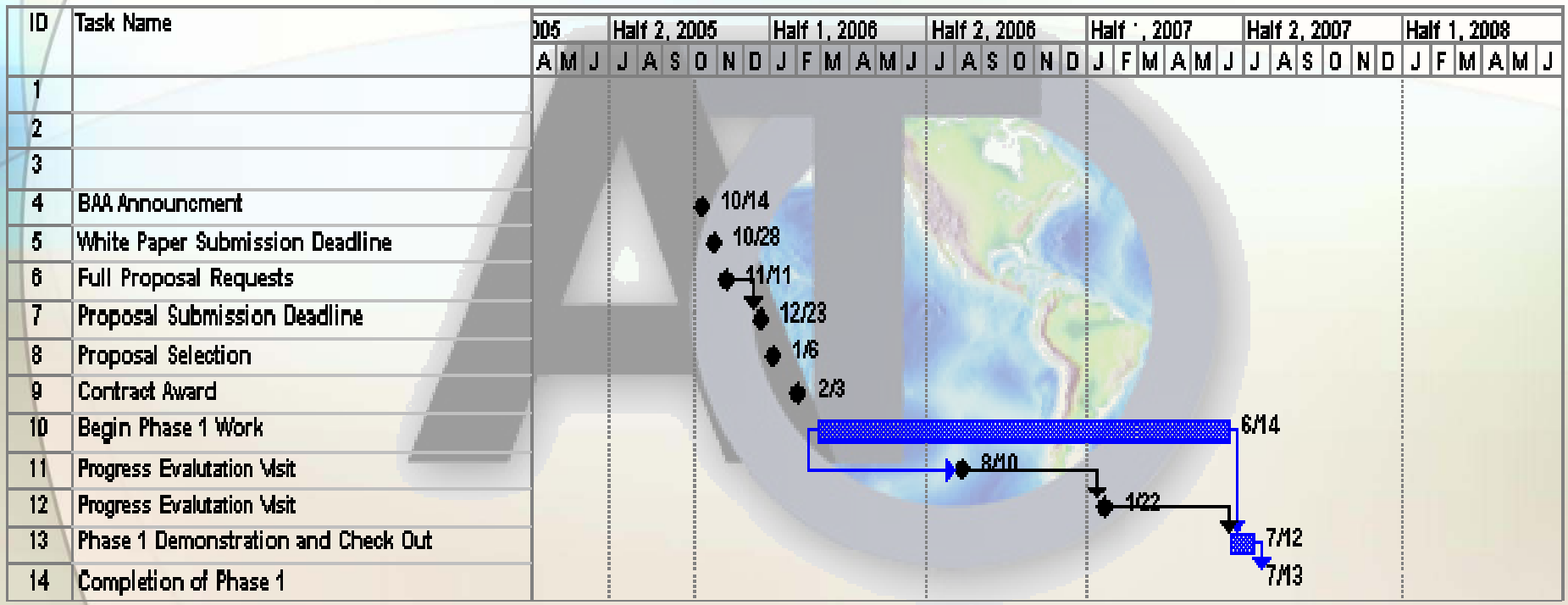
Sensitivity- <= 100 PPT in atmospheric background
PD > 1-10E^{-4}
PFA- <10E^{-4} (in atmospheric clutter described above)
Simultaneous Analyte Assays - > 30
Size - < 1 m^3 (table top unit)
Weight - < 100 lbs.
Power Consumption < 100 Watts
Required Demonstration: Correctly identify components of a mixture provided by a DoD monitor
Mission life – indeterminate, at this point
Analysis time < 10 minutes
Target unit costs < $25,000 for this stage of development

<u>Deliverables</u>

- **Develop and produce a "breadboard" level system capable of demonstrating a chemical analysis performance capability according to the specifications given above. A test sample will be provided for real-time analysis as described in Program Objectives and Description, above, as part of the proof-of-concept requirement.**
- **Compliance with all the aforementioned specifications.**
- **Provide ROC curve characterization of system performance.**
  - **To include target analyte in cluttered background.**
- **Provide signal processing of provided sample spectra depicting systems performance capability.**
- **Provide all design specifications and documentation.**

MACS Schedule and Milestones

Critical Dates -



{Note: this schedule is outdated; reference BAA and PIP for period of performance information}

Part 2. Specific Information

Mission-Adaptable Chemical Spectrometer (MACS)

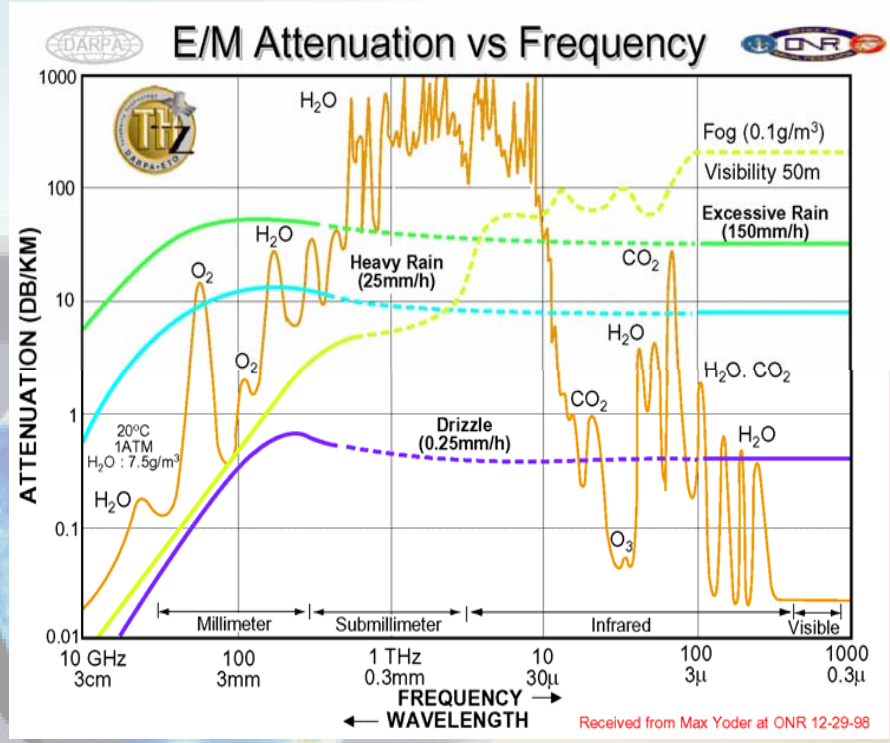
- **Objective: Build a chemical sensor that is portable (<1ft.3, <30 lbs., <25 watts total power), with sensitivity and analytical capability to identify a variety of probable Chem./Bio./Explosive threats.**

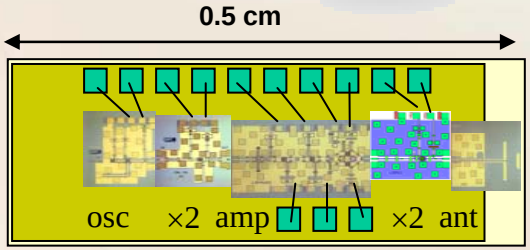
- **Assumptions: Threats can be uniquely identified by their ambient complex gas mixture. A portable chemical sensor could be built to identify this suite of constituents (up to 300 analytes), sensitively (ppt) within atmospheric clutter, quickly (<10 minutes) and uniquely associate it with a particular threat.**

- **Action: Utilize terahertz absorption spectroscopy, and solid-state components now available in this regime, to build a uniquely sensitive and discriminating sensor for dilute gases.**

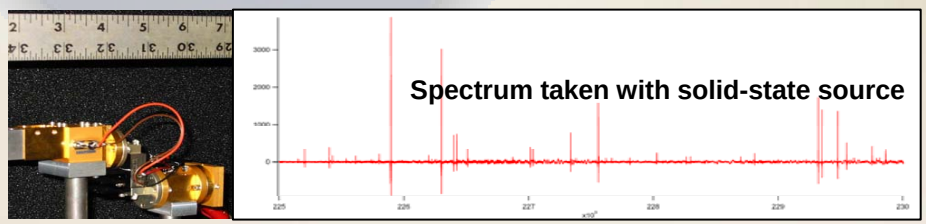
Advantages of the Terahertz Regime

- Small Doppler limit and the complex rotational fingerprint of molecules leads to absolute specificity even in complex mixtures.
- Optimum sample pressure is low and very small samples are required.
- The absorption strength peaks in the THz.
- The same physics which results in the strong atmospheric absorption also provides great sensitivity.
- Dramatic reduction in size of terahertz sources is taking place.





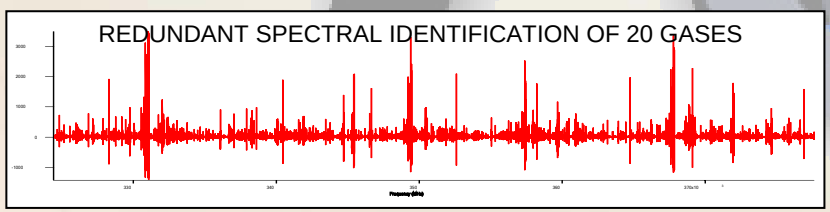
Active DARPA THz Source Development (HRL)

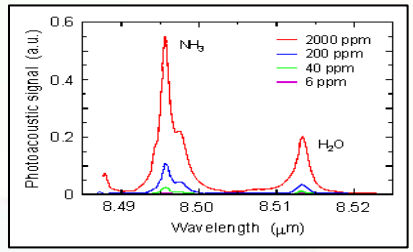


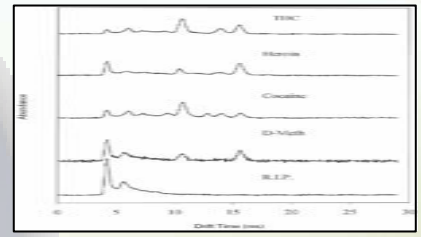
Interim Scale that Exists in the Laboratory Today

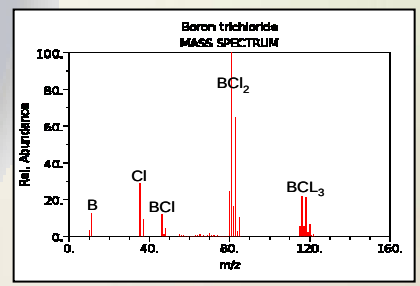
Identification Elements for Different Sensors

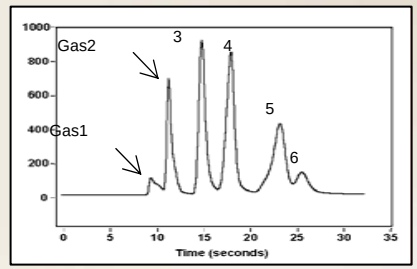
Chemical sensor Technologies	**Identification Elements for Each Sensor (based on resolution)**
Photo-Acoustic (IR)	**~200**
Gas Chromatography	**~100**
Mass Spectra	**~500**
Ion mobility	**~50**
MACS Rotational Spectra	~500,000









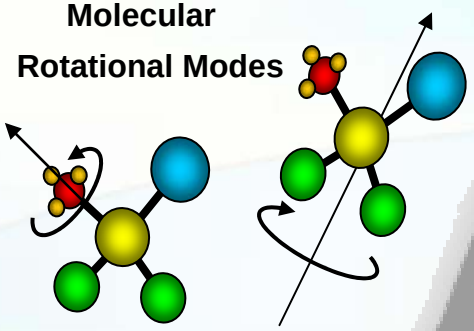


Advantages of Terahertz based rotational spectroscopy:

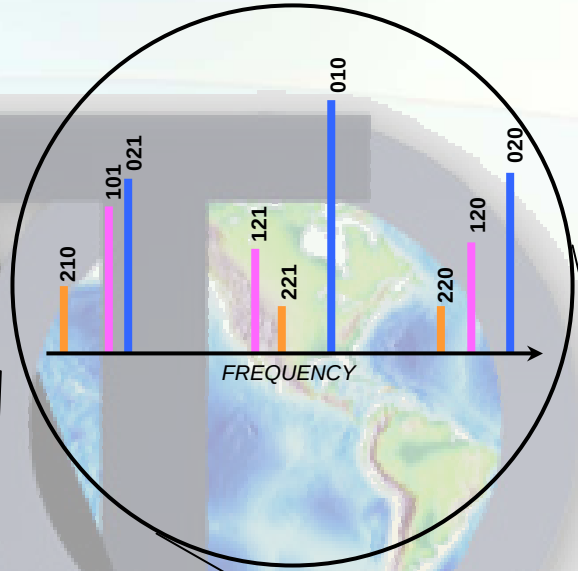
- Huge number of identifying lines
- Nearly 99% of the atmospheric clutter is ***transparent*** to THz rotational spectroscopy
- Quick identification of hundreds of chemical components.

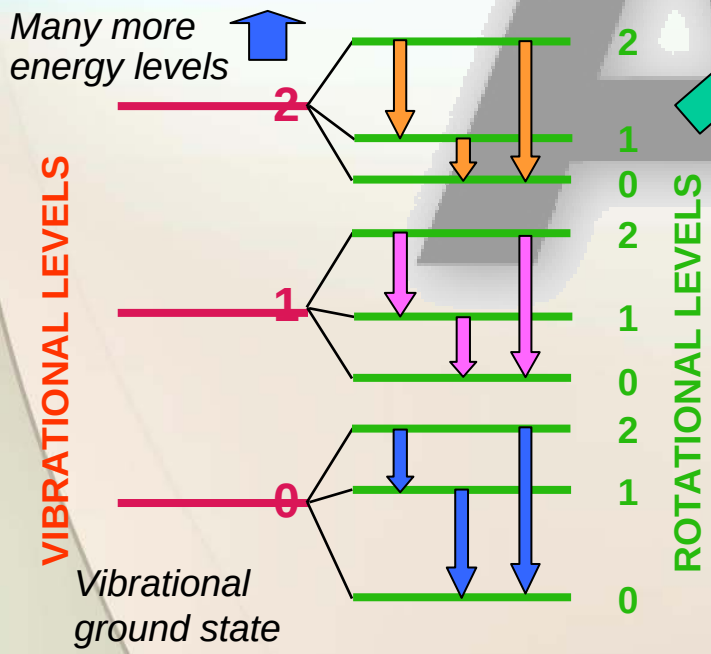
Rotational Energy Levels and Transitions

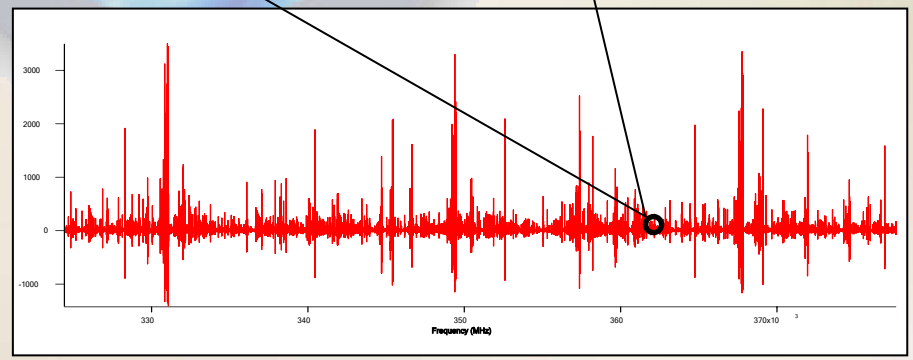
Molecular
Rotational Modes



Spectra of First Three Sets of Transitions

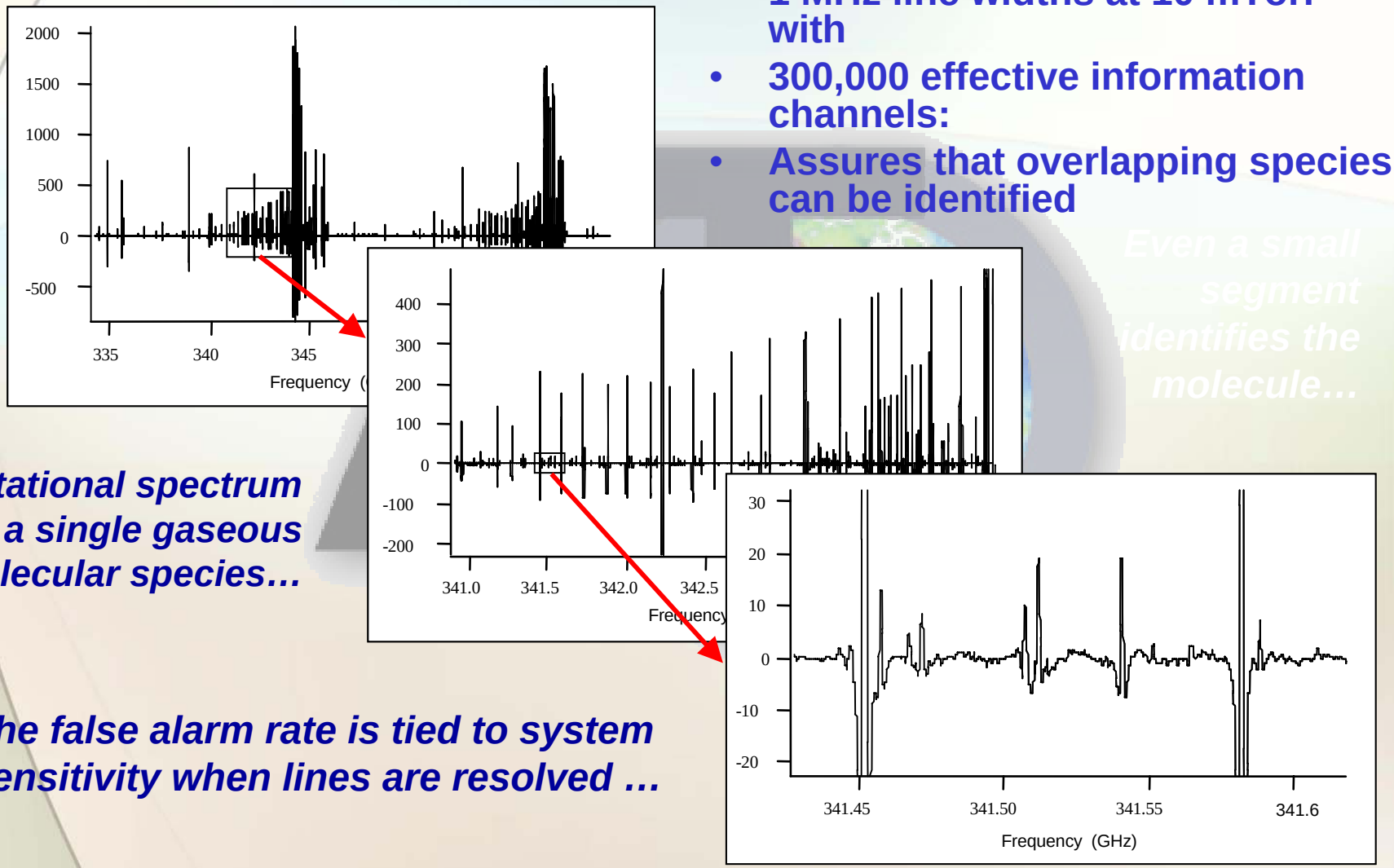






Unique Species Identification

- 1 MHz line widths at 10 mTorr with
- 300,000 effective information channels:
- Assures that overlapping species can be identified



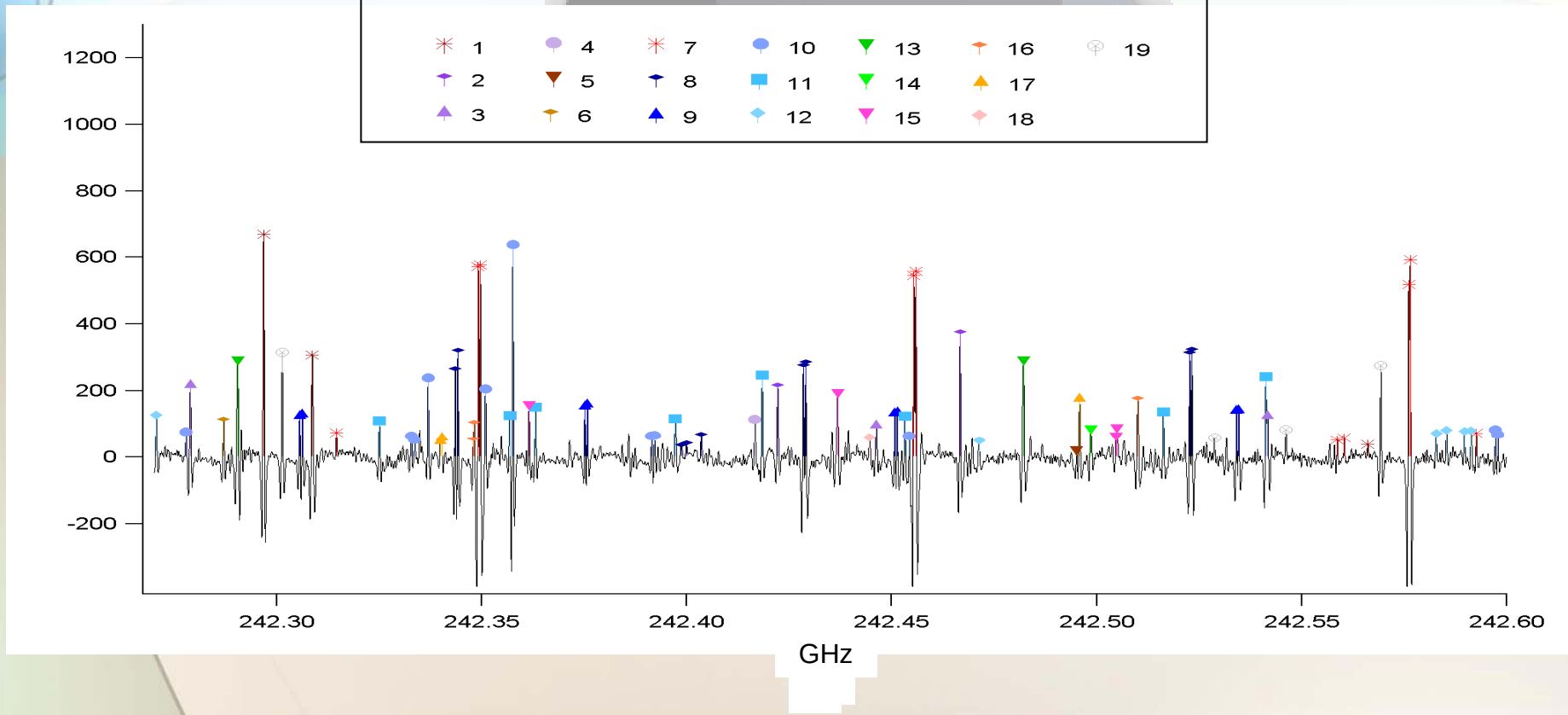
Rotational spectrum for a single gaseous molecular species…

Even a small segment identifies the molecule…

The false alarm rate is tied to system sensitivity when lines are resolved …

Absolute Identification in Complex Chemical Environment

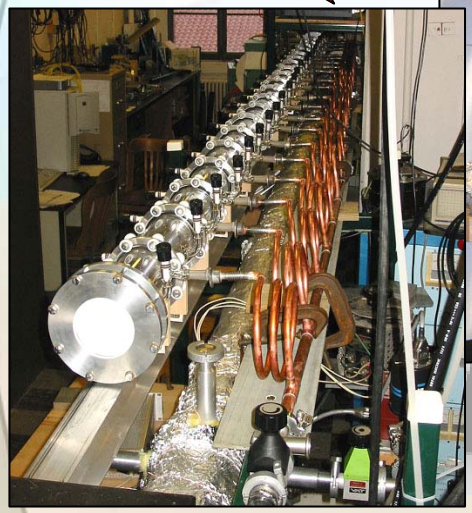
- *19 different "species"*
  - *Only 2% of 2 second scan shown - 0.01 s of data in this plot*
  - *Many other similar 10 ms subscans could have been selected*
  - *Mix of species represents a "near worst case scenario"*



Blind Test of Sensor Capability

(on Laboratory-Scale Equipment)

Showed MACS simulation can accurately identify chemicals within a complex mixture. **AFRL selected 19 chemicals (unknown to testing team) out of 30, for a BLIND TEST:**



AFRL/Contractor team installed the gases into the spectrometer and performed a sweep of the spectrum

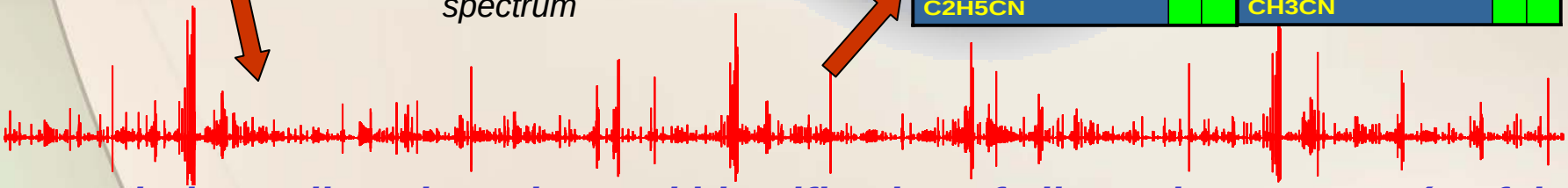
Key

T=Chemical Actually Present ("truth")

O=Chemical Observed in Mixture

Present | Not Present

Species	*T*	*O*	*Species*	*T*	*O*
CH3Cl			Methanol		
CH3Br			H2S		
CH3I			C2H5OH		
Acrolein			Methanethiol		
Oxetain			Formic Acid		
Thietain			CH2F2		
Thiophene			Acrylonitrile		
Vinyl Bromide			Vinyl Chloride		
Ethylene Oxide			CH2CF2		
CF3H			N2O		
Triflouroethane			OCS		
Thionyl Flouride			BrCN		
Vinyl Flouride			CH3F		
Carbonyl Flouride			Propyne		
C2H5CN			CH3CN		



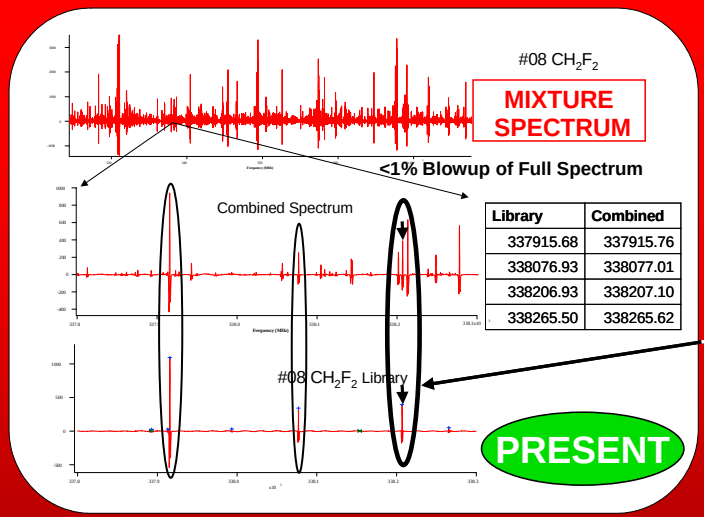
Result: immediate detection and identification of all species present (no false positives and no missed detections).

Analysis of Overlapping Spectra

NOAA "Atmospheres"

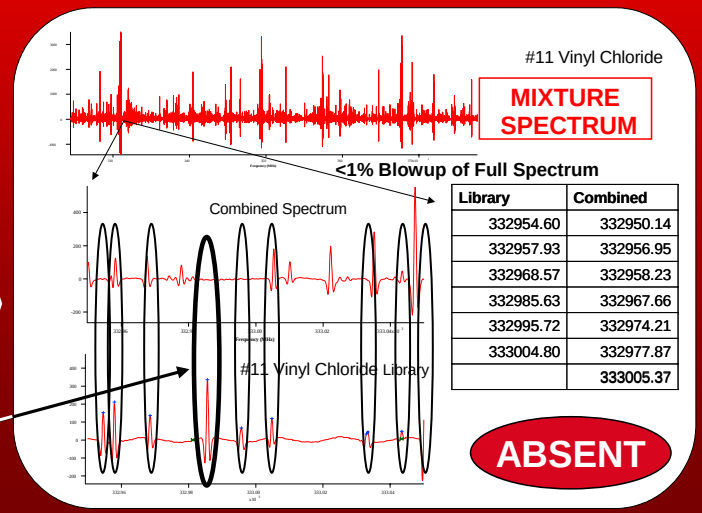
Species	New York	ASSEKREM, Algeria	South Pole, Antarctica	Trans-Siberian Railway, Russia	Harvard Forest, Massachusetts
CFC-113	2.8 ppb				
CH3CCl3	8.8 ppb				
HCFC-141b	~2.1 ppb				
CFC-11	31.5 ppb				
HCFC-142b	~1.7 ppb				
HFC-134a	~2.9 ppb				
HCFC-22	18 ppb				
CFC-12	49.8 ppb				
Halon-1301	?				
Halon-1211	~.4 ppb				
CO	1 ppm				
H2O	sparse				
NO2	0.04 ppm				
SO2	0.009 ppm				
N2O	325 ppb				
CCl4	683 ppt				
PAN	4.913 ppm				
NO	0.05 ppm				
NOy	1 ppm				
SF6	5.3 ppb				
CO2	symmetric				
H2	symmetric				
CH4	symmetric				
CH2Cl2	~4.7 ppb				
CHCl3	~1 ppb				
CH3Cl	~52 ppb				
COS	~44 ppb				
PCE					
MC	~4 ppb				
O3					
C2Cl4	~1.4 ppb				
C2HCl3	~0.2 ppb				
CH3Br	~0.7ppb				

Example of Spectral Identification/Detection



Visual examination of less than 1% of the spectral data shows the spectral precision and massive redundancy that provide the basis for MACS' 'absolute' specificity and outstanding ROCs.

A matching analyte (CH_2F_2) line



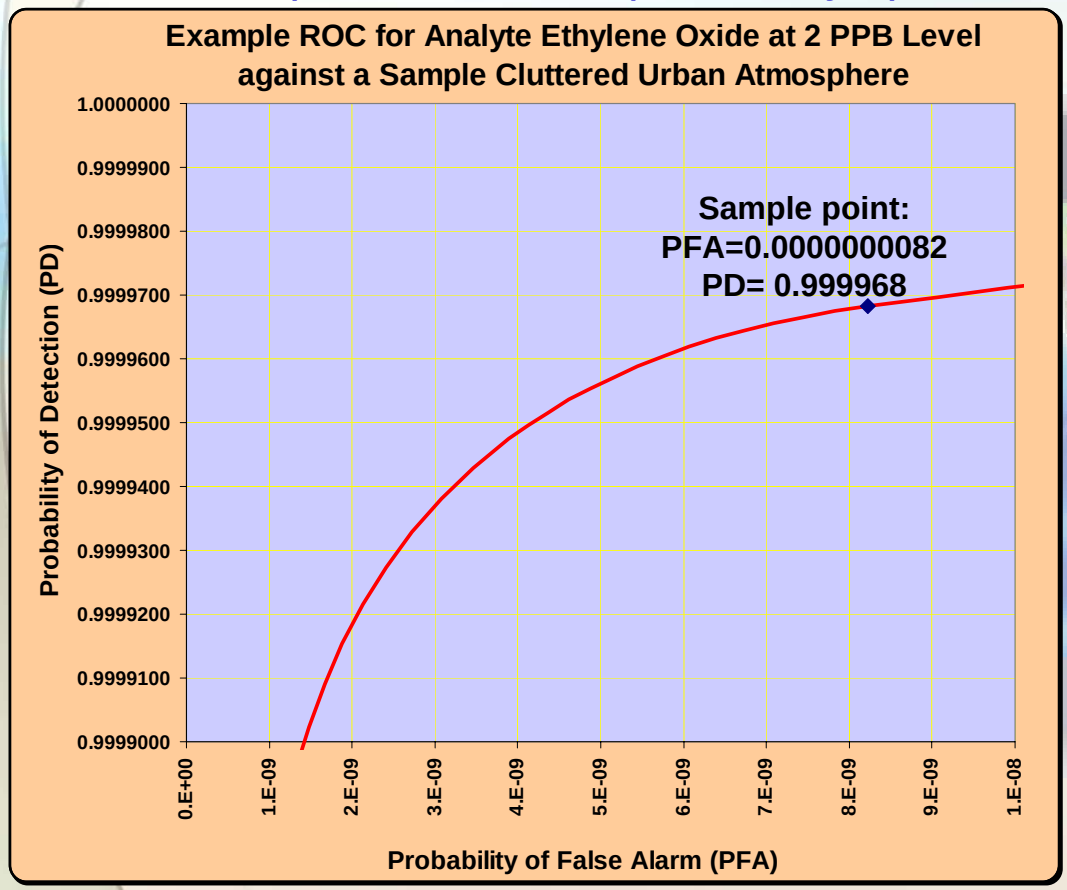
SPECIES IS PRESENT

SPECIES IS NOT PRESENT

Instance of the absence of analyte (vinyl chloride) line

MACS ROC Curve in Atmospheric Clutter

- Develop Receiver Operating Characteristic (ROC) curve in atmospheric clutter for present sensor (laboratory spectrometer), using NOAA samples,



- **Spectroscopy achieved on analyte in NOAA atmospheric samples, using available pre-MACS THz system.**

- **These results indicate that MACS can achieve reliable detection (PD > 0.99, PFA < 0.01) at *10 ppt* concentra-tion of analyte.**

Result: First ROC curve determined for analyte in atmospheric clutter, based on present laboratory system; projection for functional MACS system.

Sensor Building Blocks

Early Predictions (1955)

MICROWAVE SPECTROSCOPY

C. H. TOWNES

Professor of Physics
Columbia University

A. L. SCHAWLOW

Bell Telephone Laboratories

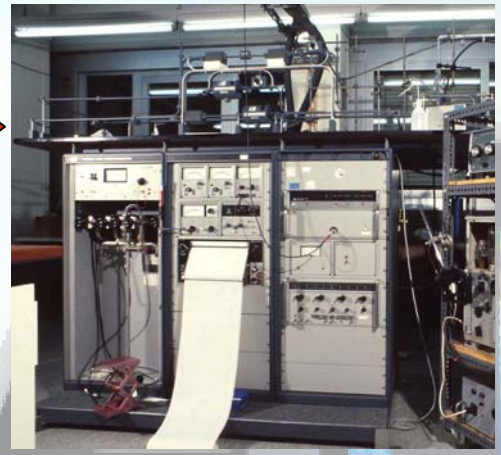
CHAPTER 18

THE USE OF MICROWAVE SPECTROSCOPY FOR CHEMICAL ANALYSIS

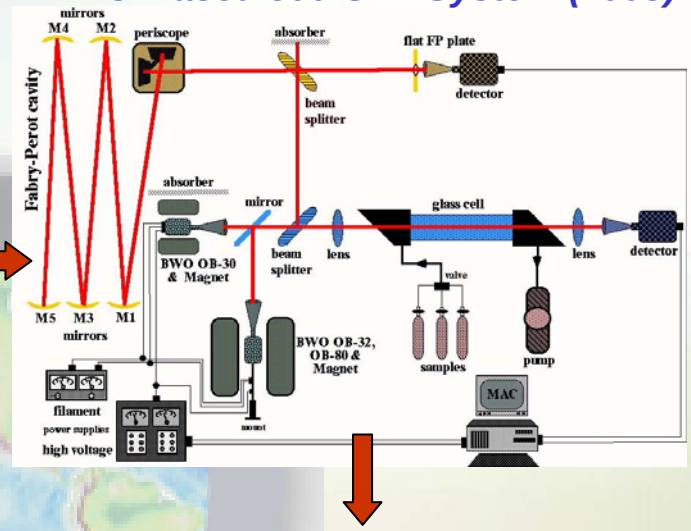
The well-known varieties of spectroscopy have been so widely and successfully used for chemical analysis that the reader has undoubtedly already wondered whether or not microwave spectroscopy can also be successfully applied in this way. Although microwave spectroscopy appears to be well suited for certain varieties of analytical work, actual applications of this type have so far been very limited.

McGRAW-HILL BOOK COMPANY, INC.
New York Toronto London
1955

40 GHz Spectrometer (1974)



BWO-Based 300 GHz System (1998)



Microfabrication (2004)

Raytheon

RMPA39200

37-40 GHz 1.6 Watt Power Amplifier MMIC

PRODUCT INFORMATION

Description

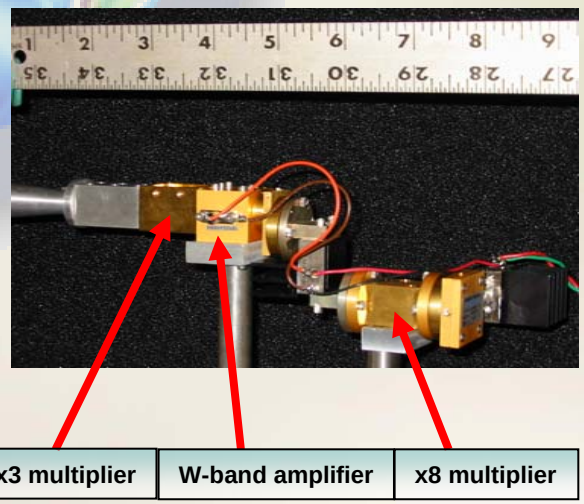
The Raytheon RMPA39200 is a high efficiency power amplifier designed for use in point to point radio, point to multi-point communications, LMDS and other millimeter wave applications. The RMPA39200 is a 3-stage GaAs MMIC amplifier utilizing Raytheon's advanced 0.15µm gate length Power PHEMT process and can be used in conjunction with other driver or power amplifiers to achieve the required total power output.

Features

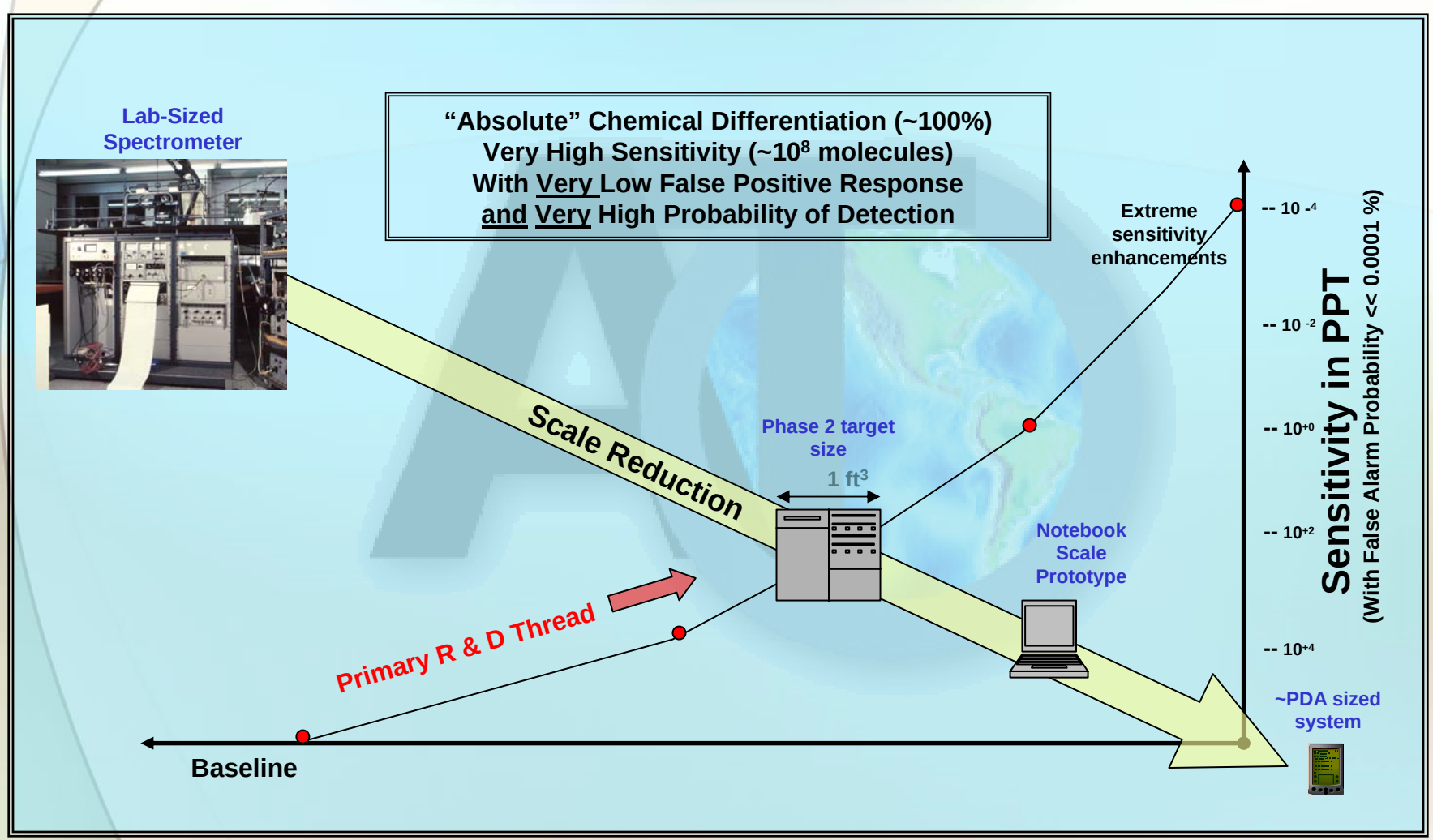
- 19 dB small signal gain (typ.)
- 32 dBm power out (typ.)
- Circuit contains individual source vias
- Chip Size 4.28 mm x 3.19 mm

- *Growth in computing power to rapidly handle information*
- *Broadband wireless market-driven technology expansion*

Solid-State Waveguide Components (2001)



MACS Program - Overview



Mission-Adaptable Chemical Spectrometer (MACS)

- **Questions concerning this proposal can be forwarded to BAA06-01@darpa.mil**
- **Please check the MACS website for FAQs (updated periodically)**

http://www.darpa.mil/ato/solicit/MACS/index.htm